

frac. valid SMILES

0.75
0.50
0.25

frac. unique SMILES

1.0
0.5

frac. SMILES in train

0.05
0.00
-0.05

frac. SMILES in PubChem

1.00
0.98

KLD
0.8
0.6

Frechet distance

50
25

frac. SMILES with azo

1
0

SA score

3.25
3.00
2.75

0.0 0.5 1.0 1.5 2.0
temperature

